

10/ 040,319

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1 Web Page URLs for STN Seminar Schedule - N. America  
NEWS 2 Apr 08 "Ask CAS" for self-help around the clock  
NEWS 3 Apr 09 BEILSTEIN: Reload and Implementation of a New Subject Area  
NEWS 4 Apr 09 ZDB will be removed from STN  
NEWS 5 Apr 19 US Patent Applications available in IFICDB, IFIPAT, and IFIUDB  
NEWS 6 Apr 22 Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS  
NEWS 7 Apr 22 BIOSIS Gene Names now available in TOXCENTER  
NEWS 8 Apr 22 Federal Research in Progress (FEDRIP) now available  
NEWS 9 Jun 03 New e-mail delivery for search results now available  
NEWS 10 Jun 10 MEDLINE Reload  
NEWS 11 Jun 10 PCTFULL has been reloaded  
NEWS 12 Jul 02 FOREGE no longer contains STANDARDS file segment  
NEWS 13 Jul 22 USAN to be reloaded July 28, 2002;  
saved answer sets no longer valid  
NEWS 14 Jul 29 Enhanced polymer searching in REGISTRY  
NEWS 15 Jul 30 NETFIRST to be removed from STN  
NEWS 16 Aug 08 CANCERLIT reload  
NEWS 17 Aug 08 PHARMAMarketLetter(PHARMAML) - new on STN  
NEWS 18 Aug 08 NTIS has been reloaded and enhanced  
NEWS 19 Aug 19 Aquatic Toxicity Information Retrieval (AQUIRE)  
now available on STN  
NEWS 20 Aug 19 IFIPAT, IFICDB, and IFIUDB have been reloaded  
NEWS 21 Aug 19 The MEDLINE file segment of TOXCENTER has been reloaded  
NEWS 22 Aug 26 Sequence searching in REGISTRY enhanced  
NEWS 23 Sep 03 JAPIO has been reloaded and enhanced  
NEWS 24 Sep 16 Experimental properties added to the REGISTRY file  
NEWS 25 Sep 16 CA Section Thesaurus available in CAPLUS and CA  
NEWS 26 Oct 01 CASREACT Enriched with Reactions from 1907 to 1985  
NEWS 27 Oct 21 EVENTLINE has been reloaded  
NEWS 28 Oct 24 BEILSTEIN adds new search fields  
NEWS 29 Oct 24 Nutraceuticals International (NUTRACEUT) now available on STN  
NEWS 30 Oct 25 MEDLINE SDI run of October 8, 2002  
NEWS 31 Nov 18 DKILIT has been renamed APOLLIT  
NEWS 32 Nov 25 More calculated properties added to REGISTRY  
NEWS 33 Dec 02 TIBKAT will be removed from STN  
NEWS 34 Dec 04 CSA files on STN  
NEWS 35 Dec 17 PCTFULL now covers WP/PCT Applications from 1978 to date  
NEWS 36 Dec 17 TOXCENTER enhanced with additional content  
NEWS 37 Dec 17 Adis Clinical Trials Insight now available on STN  
NEWS 38 Dec 30 ISMEC no longer available  
NEWS 39 Jan 21 NUTRACEUT offering one free connect hour in February 2003  
NEWS 40 Jan 21 PHARMAML offering one free connect hour in February 2003  
NEWS 41 Jan 29 Simultaneous left and right truncation added to COMPENDEX,  
ENERGY, INSPEC  
NEWS 42 Feb 13 CANCERLIT is no longer being updated  
NEWS 43 Feb 24 METADEX enhancements  
NEWS 44 Feb 24 PCTGEN now available on STN  
NEWS 45 Feb 24 TEMA now available on STN  
NEWS 46 Feb 26 NTIS now allows simultaneous left and right truncation  
NEWS 47 Feb 26 PCTFULL now contains images

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NEWS 48 Mar 04 SDI PACKAGE for monthly delivery of multifile SDI results  
NEWS 49 Mar 19 APOLLIT offering free connect time in April 2003  
NEWS 50 Mar 20 EVENTLINE will be removed from STN  
NEWS 51 Mar 24 PATDPAFULL now available on STN  
NEWS 52 Mar 24 Additional information for trade-named substances without  
structures available in REGISTRY  
NEWS 53 Mar 24 Indexing from 1957 to 1966 added to records in CA/CAPLUS

NEWS EXPRESS	January 6 CURRENT WINDOWS VERSION IS V6.01a, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 01 OCTOBER 2002
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 10:39:40 ON 31 MAR 2003

FILE 'REGISTRY' ENTERED AT 10:39:58 ON 31 MAR 2003  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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STRUCTURE FILE UPDATES: 30 MAR 2003 HIGHEST RN 500991-80-0  
DICTIONARY FILE UPDATES: 30 MAR 2003 HIGHEST RN 500991-80-0

**TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002**

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See **HELP CROSSOVER** for details.

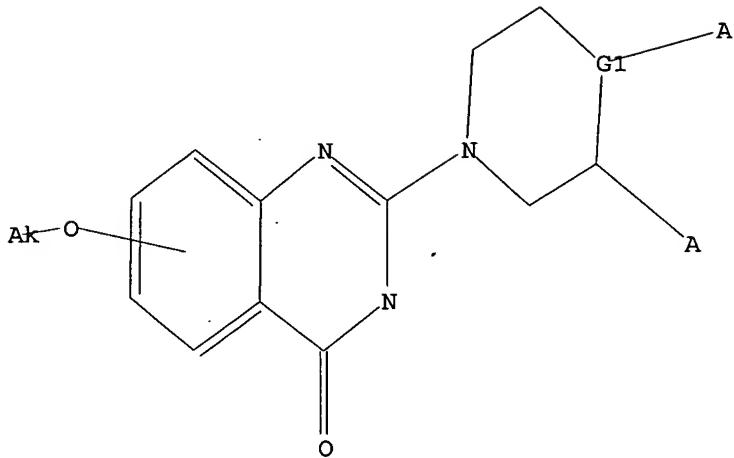
Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>  
Uploading 10040319.str

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L1 STRUCTURE UPLOADED

=> d l1  
L1 HAS NO ANSWERS  
L1 STR



G1 C,N

Structure attributes must be viewed using STN Express query preparation.

=> s l1  
SAMPLE SEARCH INITIATED 10:40:20 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 278 TO ITERATE  
  
100.0% PROCESSED 278 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01  
  
FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 4560 TO 6560  
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 ful  
FULL SEARCH INITIATED 10:40:30 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 5942 TO ITERATE  
  
100.0% PROCESSED 5942 ITERATIONS 9 ANSWERS  
SEARCH TIME: 00.00.01

L3 9 SEA SSS FUL L1

=> file caplus  
COST IN U.S. DOLLARS SINCE FILE TOTAL  
ENTRY SESSION  
FULL ESTIMATED COST 148.15 148.36

FILE 'CAPLUS' ENTERED AT 10:40:38 ON 31 MAR 2003  
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FILE COVERS 1907 - 31 Mar 2003 VOL 138 ISS 14  
FILE LAST UPDATED: 30 Mar 2003 (20030330/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> s 13
L4          0 L3

=> s caold
L5          3 CAOLD

=> file caold
COST IN U.S. DOLLARS
FULL ESTIMATED COST
```

	SINCE FILE ENTRY	TOTAL SESSION
	2.56	150.92

FILE 'CAOLD' ENTERED AT 10:41:37 ON 31 MAR 2003
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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

```
=> s 13
L6          0 L3

=> d his

(FILE 'HOME' ENTERED AT 10:39:40 ON 31 MAR 2003)
```

FILE 'REGISTRY' ENTERED AT 10:39:58 ON 31 MAR 2003
L1 STRUCTURE UPLOADED
L2 0 S L1
L3 9 S L1 FUL

FILE 'CAPLUS' ENTERED AT 10:40:38 ON 31 MAR 2003
L4 0 S L3
L5 3 S CAOLD

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FILE 'CAOLD' ENTERED AT 10:41:37 ON 31 MAR 2003  
L6 0 S L3

=> file reg  
COST IN U.S. DOLLARS  
FULL ESTIMATED COST

	SINCE FILE ENTRY	TOTAL SESSION
	0.40	151.32

FILE 'REGISTRY' ENTERED AT 10:42:11 ON 31 MAR 2003  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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Property values tagged with IC are from the ZIC/VINITI data file  
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STRUCTURE FILE UPDATES: 30 MAR 2003 HIGHEST RN 500991-80-0  
DICTIONARY FILE UPDATES: 30 MAR 2003 HIGHEST RN 500991-80-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP  
PROPERTIES for more information. See STNote 27, Searching Properties  
in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> d 13 1- ibib abs hitstr  
'IBIB' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'  
'ABS' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'  
'HITSTR' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual  
fields or predefined formats. The predefined substance formats  
are: (RN = CAS Registry Number)

REG - RN  
SAM - Index Name, MF, and structure - no RN  
FIDE - All substance data, except sequence data  
IDE - FIDE, but only 50 names  
SQIDE - IDE, plus sequence data  
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used  
SQD - Protein sequence data, includes RN  
SQD3 - Same as SQD, but 3-letter amino acid codes are used  
SQN - Protein sequence name information, includes RN  
  
CALC - Table of calculated properties  
EPROP - Table of experimental properties  
PROP - EPROP and CALC

Any CA File format may be combined with any substance format to  
obtain CA references citing the substance. The substance formats  
must be cited first. The CA File predefined formats are:

ABS -- Abstract  
APPS -- Application and Priority Information

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BIB -- CA Accession Number, plus Bibliographic Data  
CAN -- CA Accession Number  
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)  
IND -- Index Data  
IPC -- International Patent Classification  
PATS -- PI, SO  
STD -- BIB, IPC, and NCL

IABS --ABS, indented, with text labels  
IBIB -- BIB, indented, with text labels  
ISTD -- STD format, indented  
  
OBIB ----- AN, plus Bibliographic Data (original)  
OIBIB ----- OBIB, indented with text labels  
  
SBIB ----- BIB, no citations  
SIBIB ----- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.

The MAX format is the same as ALL.

The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

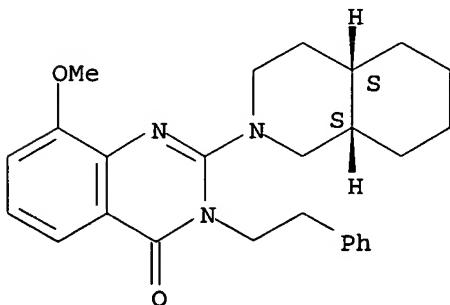
For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.  
HELP FORMATS -- To see detailed descriptions of the predefined formats.  
ENTER DISPLAY FORMAT (IDE):reg sam fide  
YOU HAVE REQUESTED DATA FROM 9 ANSWERS - CONTINUE? Y/(N):y

1           RN           319912-81-7    REGISTRY

L3    ANSWER 1 OF 9    REGISTRY    COPYRIGHT 2003 ACS  
IN    4 (3H) -Quinazolinone, 8-methoxy-2-[(4aR,8aR) -octahydro-2(1H) -isoquinolinyl] -  
      3 - (2-phenylethyl) -, rel- (9CI)  
MF    C26 H31 N3 O2

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

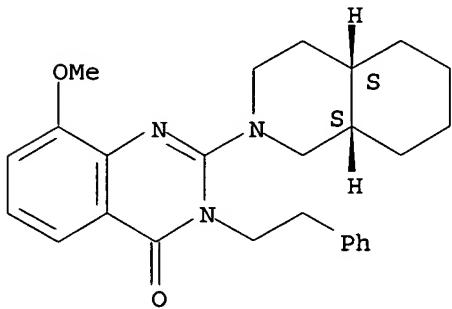
RN    319912-81-7    REGISTRY  
CN    4 (3H) -Quinazolinone, 8-methoxy-2-[(4aR,8aR) -octahydro-2(1H) -isoquinolinyl] -  
      3 - (2-phenylethyl) -, rel- (9CI)    (CA INDEX NAME)  
FS    STEREORESEARCH  
MF    C26 H31 N3 O2

SR Chemical Library  
 LC STN Files: CHEMCATS

## Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	1
C5N-C6	NC5-C6	6-6	C9N	591.50.1	1
C4N2-C6	NCNC3-C6	6-6	C8N2	591.100.37	1

Relative stereochemistry.



## Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	458	pH 1	(1) ACD
Bioconc. Factor (BCF)	2123	pH 4	(1) ACD
Bioconc. Factor (BCF)	2128	pH 7	(1) ACD
Bioconc. Factor (BCF)	2128	pH 8	(1) ACD
Bioconc. Factor (BCF)	2128	pH 10	(1) ACD
Boiling Point (BP)	577.7+/-50.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	86.48+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	303.2+/-54.2 deg C		(1) ACD
H acceptors (HAC)	5		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	1805	pH 1	(1) ACD
Koc (KOC)	8364	pH 4	(1) ACD
Koc (KOC)	8385	pH 7	(1) ACD
Koc (KOC)	8385	pH 8	(1) ACD
Koc (KOC)	8385	pH 10	(1) ACD
logD (LOGD)	4.01	pH 1	(1) ACD
logD (LOGD)	4.68	pH 4	(1) ACD
logD (LOGD)	4.68	pH 7	(1) ACD
logD (LOGD)	4.68	pH 8	(1) ACD
logD (LOGD)	4.68	pH 10	(1) ACD
logP (LOGP)	4.682+/-0.941		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD

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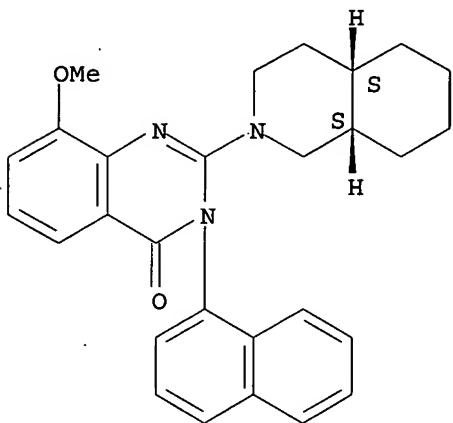
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	417.54		(1) ACD
pKa (PKA)	1.26+/-0.20	Most Basic	(1) ACD
Vapor Pressure (VP)	2.40E-13 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 ((C) 1994-2003 ACD)

2 RN 319912-77-1 REGISTRY

L3 ANSWER 2 OF 9 REGISTRY COPYRIGHT 2003 ACS  
IN 4 (3H)-Quinazolinone, 8-methoxy-3-(1-naphthalenyl)-2-[(4aR,8aR)-octahydro-2 (1H)-isoquinolinyl]-, rel- (9CI)  
MF C28 H29 N3 O2

Relative stereochemistry.



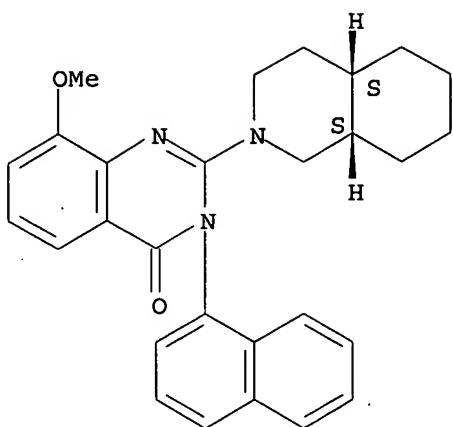
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

RN 319912-77-1 REGISTRY  
CN 4 (3H)-Quinazolinone, 8-methoxy-3-(1-naphthalenyl)-2-[(4aR,8aR)-octahydro-2 (1H)-isoquinolinyl]-, rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C28 H29 N3 O2  
SR Chemical Library  
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID	Occurrence Count
EA	ES	SZ	RF	RID		
C6-C6	C6-C6	6-6	C10	591.49.57	1	
C5N-C6	NC5-C6	6-6	C9N	591.50.1	1	
C4N2-C6	NCNC3-C6	6-6	C8N2	591.100.37	1	

Relative stereochemistry.



## Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	6810	pH 1	(1) ACD
Bioconc. Factor (BCF)	8484	pH 4	(1) ACD
Bioconc. Factor (BCF)	8486	pH 7	(1) ACD
Bioconc. Factor (BCF)	8486	pH 8	(1) ACD
Bioconc. Factor (BCF)	8486	pH 10	(1) ACD
Boiling Point (BP)	617.6+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	91.58+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	327.3+/-56.7 deg C		(1) ACD
H acceptors (HAC)	5		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	18110	pH 1	(1) ACD
Koc (KOC)	22562	pH 4	(1) ACD
Koc (KOC)	22568	pH 7	(1) ACD
Koc (KOC)	22568	pH 8	(1) ACD
Koc (KOC)	22568	pH 10	(1) ACD
logD (LOGD)	5.38	pH 1	(1) ACD
logD (LOGD)	5.47	pH 4	(1) ACD
logD (LOGD)	5.47	pH 7	(1) ACD
logD (LOGD)	5.47	pH 8	(1) ACD
logD (LOGD)	5.47	pH 10	(1) ACD
logP (LOGP)	5.473+/-0.940		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	439.55		(1) ACD
pKa (PKA)	0.36+/-0.70	Most Basic	(1) ACD
Vapor Pressure (VP)	3.49E-15 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 ((C) 1994-2003 ACD)

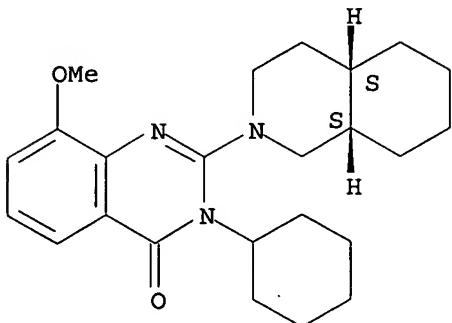
3 RN 319912-71-5 REGISTRY

L3 ANSWER 3 OF 9 REGISTRY COPYRIGHT 2003 ACS  
 IN 4-(3H)-Quinazolinone, 3-cyclohexyl-8-methoxy-2-[(4aR,8aR)-octahydro-2(1H)-

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isoquinolinyl]-, rel- (9CI)  
MF C24 H33 N3 O2

Relative stereochemistry.



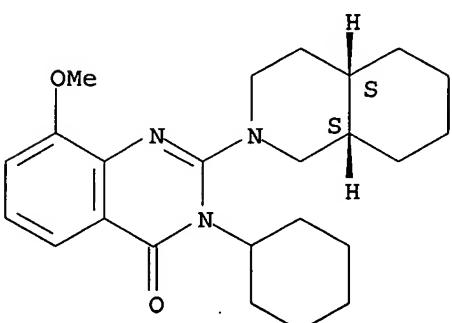
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

RN 319912-71-5 REGISTRY  
CN 4 (3H)-Quinazolinone, 3-cyclohexyl-8-methoxy-2-[(4aR,8aR)-octahydro-2(1H)-isoquinolinyl]-, rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C24 H33 N3 O2  
SR Chemical Library  
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID
EA	ES	SZ	RF	RID	Occurrence Count
C6	C6	6	C6	46.150.1	1
C5N-C6	NC5-C6	6-6	C9N	591.50.1	1
C4N2-C6	NCNC3-C6	6-6	C8N2	591.100.37	1

Relative stereochemistry.



## Calculated Properties (CALC)

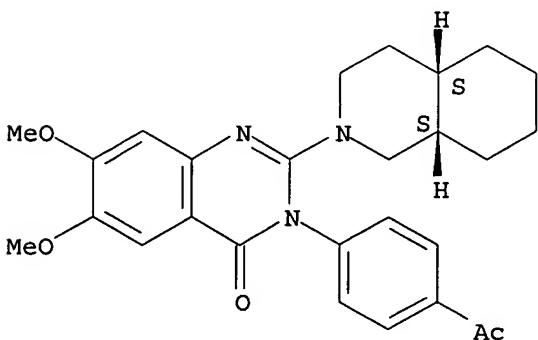
PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	318	pH 1	(1) ACD
Bioconc. Factor (BCF)	1682	pH 4	(1) ACD
Bioconc. Factor (BCF)	1687	pH 7	(1) ACD
Bioconc. Factor (BCF)	1687	pH 8	(1) ACD
Bioconc. Factor (BCF)	1687	pH 10	(1) ACD
Boiling Point (BP)	542.7+/-50.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	82.09+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	282.0+/-54.2 deg C		(1) ACD
H acceptors (HAC)	5		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	1336	pH 1	(1) ACD
Koc (KOC)	7081	pH 4	(1) ACD
Koc (KOC)	7100	pH 7	(1) ACD
Koc (KOC)	7100	pH 8	(1) ACD
Koc (KOC)	7100	pH 10	(1) ACD
logD (LOGD)	3.82	pH 1	(1) ACD
logD (LOGD)	4.55	pH 4	(1) ACD
logD (LOGD)	4.55	pH 7	(1) ACD
logD (LOGD)	4.55	pH 8	(1) ACD
logD (LOGD)	4.55	pH 10	(1) ACD
logP (LOGP)	4.550+/-0.940		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	395.54		(1) ACD
pKa (PKA)	1.30+/-0.20	Most Basic	(1) ACD
Vapor Pressure (VP)	7.71E-12 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 ((C) 1994-2003 ACD)

4 RN 318957-21-0 REGISTRY

L3 ANSWER 4 OF 9 REGISTRY COPYRIGHT 2003 ACS  
 IN 4(3H)-Quinazolinone, 3-(4-acetylphenyl)-6,7-dimethoxy-2-[(4aR,8aR)-  
 octahydro-2(1H)-isoquinolinyl]-, rel- (9CI)  
 MF C27 H31 N3 O4

Relative stereochemistry.



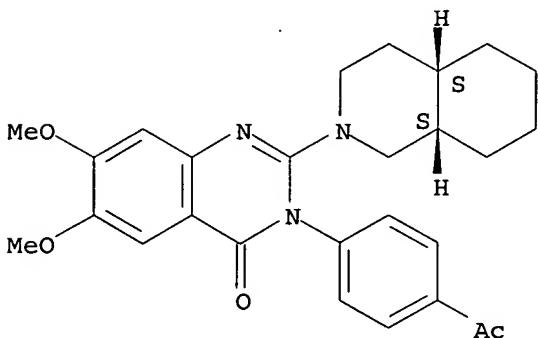
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

RN 318957-21-0 REGISTRY  
 CN 4 (3H)-Quinazolinone, 3- (4-acetylphenyl)-6,7-dimethoxy-2- [(4aR,8aR)-  
 octahydro-2(1H)-isoquinolinyl]-, rel- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C27 H31 N3 O4  
 SR Chemical Library

## Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier RID	RID Occurrence Count
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	1
C5N-C6	NC5-C6	6-6	C9N	591.50.1	1
C4N2-C6	NCNC3-C6	6-6	C8N2	591.100.37	1

## Relative stereochemistry.



## Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	717	pH 1	(1) ACD
Bioconc. Factor (BCF)	727	pH 4	(1) ACD
Bioconc. Factor (BCF)	727	pH 7	(1) ACD
Bioconc. Factor (BCF)	727	pH 8	(1) ACD
Bioconc. Factor (BCF)	727	pH 10	(1) ACD
Boiling Point (BP)	632.4 +/- 65.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	93.50 +/- 3.0 kJ/mol		(1) ACD
Flash Point (FP)	336.3 +/- 61.7 deg C		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	3833	pH 1	(1) ACD
Koc (KOC)	3887	pH 4	(1) ACD
Koc (KOC)	3887	pH 7	(1) ACD
Koc (KOC)	3887	pH 8	(1) ACD
Koc (KOC)	3887	pH 10	(1) ACD
logD (LOGD)	4.06	pH 1	(1) ACD
logD (LOGD)	4.07	pH 4	(1) ACD
logD (LOGD)	4.07	pH 7	(1) ACD
logD (LOGD)	4.07	pH 8	(1) ACD

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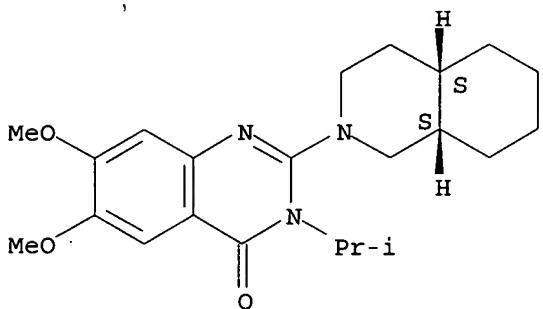
logD (LOGD)	4.07	pH 10	(1) ACD
logP (LOGP)	4.069+/-0.962		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	461.55		(1) ACD
Vapor Pressure (VP)	6.72E-16 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 ((C) 1994-2003 ACD)

5 RN 318957-19-6 REGISTRY

L3 ANSWER 5 OF 9 REGISTRY COPYRIGHT 2003 ACS  
IN 4(3H)-Quinazolinone, 6,7-dimethoxy-3-(1-methylethyl)-2-[(4aR,8aR)-  
octahydro-2(1H)-isoquinolinyl]-, rel- (9CI)  
MF C22 H31 N3 O3

Relative stereochemistry.



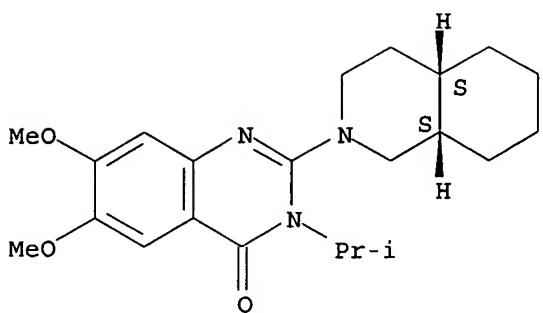
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

RN 318957-19-6 REGISTRY  
CN 4(3H)-Quinazolinone, 6,7-dimethoxy-3-(1-methylethyl)-2-[(4aR,8aR)-  
octahydro-2(1H)-isoquinolinyl]-, rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C22 H31 N3 O3  
SR Chemical Library

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID
EA	ES	SZ	RF	RID	Occurrence Count
C5N-C6	NC5-C6	6-6	C9N	591.50.1	1
C4N2-C6	NCNC3-C6	6-6	C8N2	591.100.37	1

Relative stereochemistry.



## Calculated Properties (CALC)

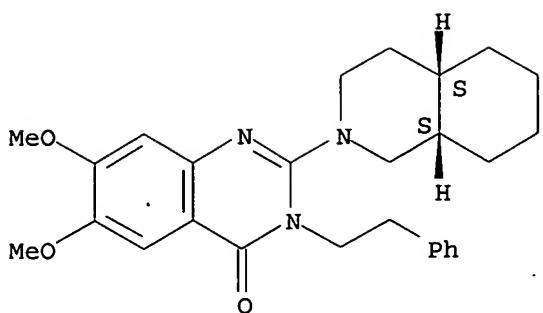
PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	25.4	pH 1	(1) ACD
Bioconc. Factor (BCF)	240	pH 4	(1) ACD
Bioconc. Factor (BCF)	242	pH 7	(1) ACD
Bioconc. Factor (BCF)	242	pH 8	(1) ACD
Bioconc. Factor (BCF)	242	pH 10	(1) ACD
Boiling Point (BP)	518.3 +/- 55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	79.08 +/- 3.0 kJ/mol		(1) ACD
Flash Point (FP)	267.3 +/- 56.7 deg C		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	185	pH 1	(1) ACD
Koc (KOC)	1756	pH 4	(1) ACD
Koc (KOC)	1770	pH 7	(1) ACD
Koc (KOC)	1770	pH 8	(1) ACD
Koc (KOC)	1770	pH 10	(1) ACD
logD (LOGD)	2.46	pH 1	(1) ACD
logD (LOGD)	3.44	pH 4	(1) ACD
logD (LOGD)	3.44	pH 7	(1) ACD
logD (LOGD)	3.44	pH 8	(1) ACD
logD (LOGD)	3.44	pH 10	(1) ACD
logP (LOGP)	3.440 +/- 0.951		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	385.50		(1) ACD
pKa (PKA)	1.91 +/- 0.20	Most Basic	(1) ACD
Vapor Pressure (VP)	7.57E-11 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 ((C) 1994-2003 ACD)

6 RN 318957-16-3 REGISTRY

L3 ANSWER 6 OF 9 REGISTRY COPYRIGHT 2003 ACS  
 IN 4(3H)-Quinazolinone, 6,7-dimethoxy-2-[(4aR,8aR)-octahydro-2(1H)-isoquinolinyl]-3-(2-phenylethyl)-, rel- (9CI)  
 MF C27 H33 N3 O3

Relative stereochemistry.



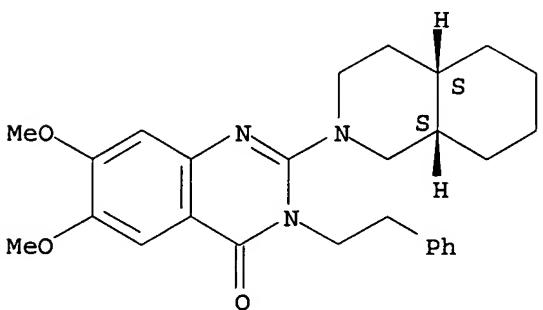
## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

RN 318957-16-3 REGISTRY  
 CN 4 (3H) -Quinazolinone, 6,7-dimethoxy-2-[(4aR,8aR)-octahydro-2(1H)-  
 isoquinolinyl]-3-(2-phenylethyl)-, rel- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C27 H33 N3 O3  
 SR Chemical Library

## Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID
EA	ES	SZ	RF	RID	Occurrence Count
C6	C6	6	C6	46.150.18	1
C5N-C6	NC5-C6	6-6	C9N	591.50.1	1
C4N2-C6	NCNC3-C6	6-6	C8N2	591.100.37	1

## Relative stereochemistry.



## Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	389	pH 1	(1) ACD
Bioconc. Factor (BCF)	2401	pH 4	(1) ACD
Bioconc. Factor (BCF)	2413	pH 7	(1) ACD
Bioconc. Factor (BCF)	2413	pH 8	(1) ACD
Bioconc. Factor (BCF)	2413	pH 10	(1) ACD

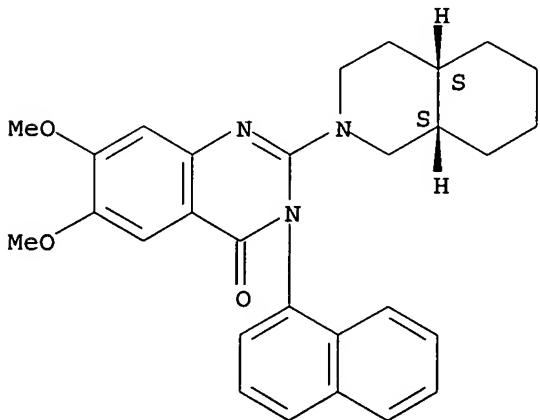
Boiling Point (BP)	604.3+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	89.86+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	319.2+/-59.2 deg C		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	1480	pH 1	(1) ACD
Koc (KOC)	9127	pH 4	(1) ACD
Koc (KOC)	9173	pH 7	(1) ACD
Koc (KOC)	9173	pH 8	(1) ACD
Koc (KOC)	9173	pH 10	(1) ACD
logD (LOGD)	3.96	pH 1	(1) ACD
logD (LOGD)	4.75	pH 4	(1) ACD
logD (LOGD)	4.75	pH 7	(1) ACD
logD (LOGD)	4.75	pH 8	(1) ACD
logD (LOGD)	4.75	pH 10	(1) ACD
logP (LOGP)	4.754+/-0.951		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	447.57		(1) ACD
pKa (PKA)	1.69+/-0.20	Most Basic	(1) ACD
Vapor Pressure (VP)	1.49E-14 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.67 ((C) 1994-2003 ACD)

7 RN 318957-14-1 REGISTRY

L3 ANSWER 7 OF 9 REGISTRY COPYRIGHT 2003 ACS  
 IN 4(3H)-Quinazolinone, 6,7-dimethoxy-3-(1-naphthalenyl)-2-[(4aR,8aR)-  
 octahydro-2(1H)-isoquinolinyl]-, rel- (9CI)  
 MF C29 H31 N3 O3

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

RN 318957-14-1 REGISTRY  
 CN 4(3H)-Quinazolinone, 6,7-dimethoxy-3-(1-naphthalenyl)-2-[(4aR,8aR)-  
 octahydro-2(1H)-isoquinolinyl]-, rel- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH

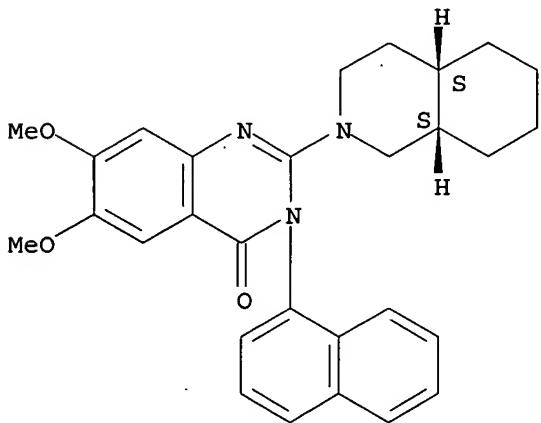
10/ 040,319

MF C29 H31 N3 O3  
SR Chemical Library

### Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C6-C6	C6-C6	6-6	C10	591.49.57	1
C5N-C6	NC5-C6	6-6	C9N	591.50.1	1
C4N2-C6	NCNC3-C6	6-6	C8N2	591.100.37	1

### Relative stereochemistry.



### Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	9082	pH 1	(1) ACD
Bioconc. Factor (BCF)	9620	pH 4	(1) ACD
Bioconc. Factor (BCF)	9621	pH 7	(1) ACD
Bioconc. Factor (BCF)	9621	pH 8	(1) ACD
Bioconc. Factor (BCF)	9621	pH 10	(1) ACD
Boiling Point (BP)	640.6+/-60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	94.58+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	341.2+/-59.2 deg C		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	23305	pH 1	(1) ACD
Koc (KOC)	24687	pH 4	(1) ACD
Koc (KOC)	24688	pH 7	(1) ACD
Koc (KOC)	24688	pH 8	(1) ACD
Koc (KOC)	24688	pH 10	(1) ACD
logD (LOGD)	5.52	pH 1	(1) ACD
logD (LOGD)	5.54	pH 4	(1) ACD
logD (LOGD)	5.54	pH 7	(1) ACD
logD (LOGD)	5.54	pH 8	(1) ACD
logD (LOGD)	5.54	pH 10	(1) ACD

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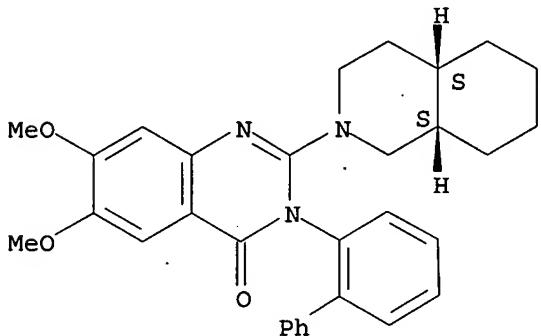
logP (LOGP)	5.545+/-0.950		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	469.57		(1) ACD
Vapor Pressure (VP)	2.62E-16 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris  
V4.67 ((C) 1994-2003 ACD)

8 RN 318957-11-8 REGISTRY

L3 ANSWER 8 OF 9 REGISTRY COPYRIGHT 2003 ACS  
IN 4(3H)-Quinazolinone, 3-[1,1'-biphenyl]-2-yl-6,7-dimethoxy-2-[(4aR,8aR)-  
octahydro-2(1H)-isoquinolinyl]-, rel- (9CI)  
MF C31 H33 N3 O3

Relative stereochemistry.



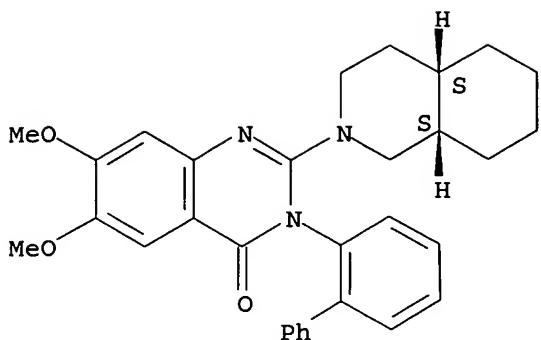
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

RN 318957-11-8 REGISTRY  
CN 4(3H)-Quinazolinone, 3-[1,1'-biphenyl]-2-yl-6,7-dimethoxy-2-[(4aR,8aR)-  
octahydro-2(1H)-isoquinolinyl]-, rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C31 H33 N3 O3  
SR Chemical Library  
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID	Occurrence Count
EA	ES	SZ	RF	RID		
C6	C6	6	C6	46.150.18	2	
C5N-C6	NC5-C6	6-6	C9N	591.50.1	1	
C4N2-C6	NCNC3-C6	6-6	C8N2	591.100.37	1	

Relative stereochemistry.



## Calculated Properties (CALC)

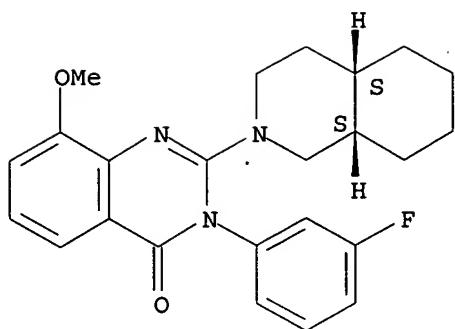
PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	23295	pH 1	(1) ACD
Bioconc. Factor (BCF)	24177	pH 4	(1) ACD
Bioconc. Factor (BCF)	24178	pH 7	(1) ACD
Bioconc. Factor (BCF)	24178	pH 8	(1) ACD
Bioconc. Factor (BCF)	24178	pH 10	(1) ACD
Boiling Point (BP)	656.7 +/- -60.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	96.69 +/- -3.0 kJ/mol		(1) ACD
Flash Point (FP)	350.9 +/- -59.2 deg C		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	46004	pH 1	(1) ACD
Koc (KOC)	47747	pH 4	(1) ACD
Koc (KOC)	47749	pH 7	(1) ACD
Koc (KOC)	47749	pH 8	(1) ACD
Koc (KOC)	47749	pH 10	(1) ACD
logD (LOGD)	6.05	pH 1	(1) ACD
logD (LOGD)	6.07	pH 4	(1) ACD
logD (LOGD)	6.07	pH 7	(1) ACD
logD (LOGD)	6.07	pH 8	(1) ACD
logD (LOGD)	6.07	pH 10	(1) ACD
logP (LOGP)	6.071 +/- -0.967		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	495.61		(1) ACD
Vapor Pressure (VP)	4.04E-17 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris  
V4.67 ((C) 1994-2003 ACD)

9 RN 318956-79-5 REGISTRY

L3 ANSWER 9 OF 9 REGISTRY COPYRIGHT 2003 ACS  
IN 4 (3H)-Quinazolinone, 3-(3-fluorophenyl)-8-methoxy-2-[(4aR,8aR)-octahydro-  
2 (1H)-isoquinolinyl]-, rel- (9CI)  
MF C24 H26 F N3 O2

Relative stereochemistry.



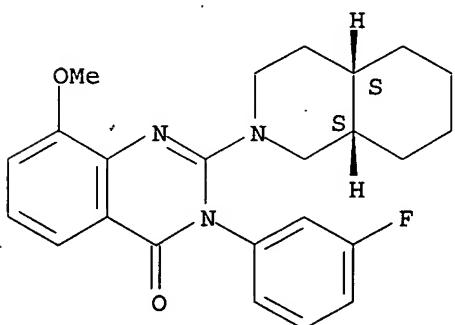
## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

RN 318956-79-5 REGISTRY  
 CN 4 (3H)-Quinazolinone, 3- (3-fluorophenyl)-8-methoxy-2- [(4aR,8aR)-octahydro-  
 2 (1H)-isoquinolinyl]-, rel- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C24 H26 F N3 O2  
 SR Chemical Library  
 LC STN Files: CHEMCATS

## Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID
EA	ES	SZ	RF	RID	Occurrence Count
C6	C6	6	C6	46.150.18	1
C5N-C6	NC5-C6	6-6	C9N	591.50.1	1
C4N2-C6	NCNC3-C6	6-6	C8N2	591.100.37	1

## Relative stereochemistry.



## Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE

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Bioconc. Factor (BCF)	1135	pH 1	(1) ACD
Bioconc. Factor (BCF)	1354	pH 4	(1) ACD
Bioconc. Factor (BCF)	1354	pH 7	(1) ACD
Bioconc. Factor (BCF)	1354	pH 8	(1) ACD
Bioconc. Factor (BCF)	1354	pH 10	(1) ACD
Boiling Point (BP)	554.3+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	83.53+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	289.0+/-56.7 deg C		(1) ACD
H acceptors (HAC)	5		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	5083	pH 1	(1) ACD
Koc (KOC)	6065	pH 4	(1) ACD
Koc (KOC)	6067	pH 7	(1) ACD
Koc (KOC)	6067	pH 8	(1) ACD
Koc (KOC)	6067	pH 10	(1) ACD
logD (LOGD)	4.35	pH 1	(1) ACD
logD (LOGD)	4.42	pH 4	(1) ACD
logD (LOGD)	4.42	pH 7	(1) ACD
logD (LOGD)	4.42	pH 8	(1) ACD
logD (LOGD)	4.42	pH 10	(1) ACD
logP (LOGP)	4.424+/-0.979		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	407.48		(1) ACD
pKa (PKA)	0.28+/-0.70	Most Basic	(1) ACD
Vapor Pressure (VP)	2.50E-12 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris  
V4.67 ((C) 1994-2003 ACD)

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and NEWS FILE for details.

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FILE 'REGISTRY' ENTERED AT 10:39:58 ON 31 MAR 2003

L1                   STRUCTURE UPLOADED  
L2                   0 S L1  
L3                   9 S L1 FUL

FILE 'CAPLUS' ENTERED AT 10:40:38 ON 31 MAR 2003

L4                   0 S L3  
L5                   3 S CAOLD

FILE 'CAOLD' ENTERED AT 10:41:37 ON 31 MAR 2003

L6                   0 S L3

FILE 'REGISTRY' ENTERED AT 10:42:11 ON 31 MAR 2003

FILE 'CHEMCATS' ENTERED AT 10:46:09 ON 31 MAR 2003

=> s 13  
L7                   5 L3

=> d 17 1- ibib abs histstr  
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'ABS' IS NOT A VALID FORMAT FOR FILE 'CHEMCATS'  
'HISTSTR' IS NOT A VALID FORMAT FOR FILE 'CHEMCATS'

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KWIC --- All hit terms plus 20 words on either side  
OCC ---- List of display fields containing hit terms

Hit terms will be highlighted in all displayable fields.

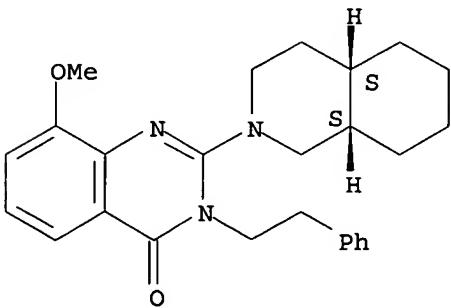
To display a particular field or fields, enter the display field codes. For a list of display field codes, enter 'HELP DFIELDS' at an arrow prompt (=>). Examples include: 'KWIC'; 'CN RN'; 'IDE CO'. You may specify the formats and fields in any order, and the information will be displayed in the same order as the format specification.

The same formats (except for HIT, KWIC, and OCC) may be used with the DISPLAY ACC command to display the record for a specified Accession Number.

ENTER DISPLAY FORMAT (IDE):all  
YOU HAVE REQUESTED DATA FROM 5 ANSWERS - CONTINUE? Y/(N):y

L7 ANSWER 1 OF 5 CHEMCATS COPYRIGHT 2003 ACS  
Accession No. (AN): 2001:187968 CHEMCATS *note*  
Catalog Name (CO): Chem.Folio  
Publication Date (PD): 15 May 2001  
Order Number (ON): TRG10400#06028-D  
Chemical Name (CN): 4(3H)-Quinazolinone, 8-methoxy-2-[(4aR,8aR)-octahydro-  
2(1H)-isoquinolinyl]-3-(2-phenylethyl)-, rel-  
CAS Registry No. (RN): 319912-81-7  
Supplementary Term (ST): CHEMICAL LIBRARY  
Structure :

Relative stereochemistry.



#### PRICES

Quantity : milligram quantities, Price: contact supplier

#### COMPANY INFORMATION

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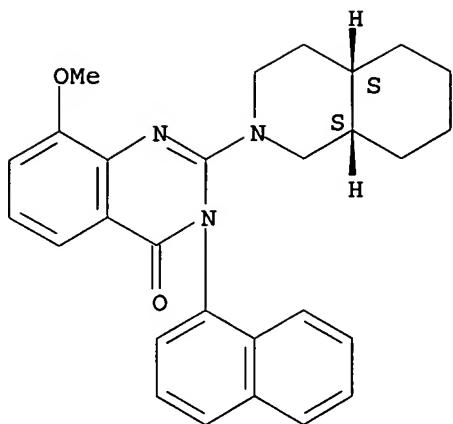
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L7 ANSWER 2 OF 5 CHEMCATS COPYRIGHT 2003 ACS  
Accession No. (AN): 2001:187964 CHEMCATS  
Catalog Name (CO): Chem.Folio  
Publication Date (PD): 15 May 2001  
Order Number (ON): TRG10400#06027-D  
Chemical Name (CN): 4 (3H) -Quinazolinone, 8-methoxy-3- (1-naphthalenyl) -2-  
[(4aR,8aR) -octahydro-2 (1H) -isoquinolinyl] -, rel-  
CAS Registry No. (RN): 319912-77-1  
Supplementary Term (ST): CHEMICAL LIBRARY  
Structure :

Relative stereochemistry.

*Colle*



PRICES

Quantity : milligram quantities, Price: contact supplier

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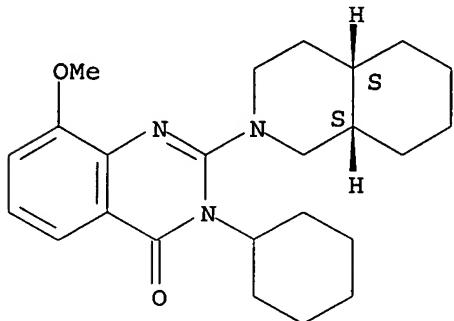
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L7 ANSWER 3 OF 5 CHEMCATS COPYRIGHT 2003 ACS  
Accession No. (AN) : 2001:187958 CHEMCATS  
Catalog Name (CO) : Chem.Folio  
Publication Date (PD) : 15 May 2001  
Order Number (ON) : TRG10400#06025-D  
Chemical Name (CN) : 4 (3H)-Quinazolinone, 3-cyclohexyl-8-methoxy-2-[ (4aR,8aR)-octahydro-2(1H)-isoquinolinyl] -, rel-  
CAS Registry No. (RN) : 319912-71-5  
Supplementary Term (ST) : CHEMICAL LIBRARY  
Structure :

Relative stereochemistry.



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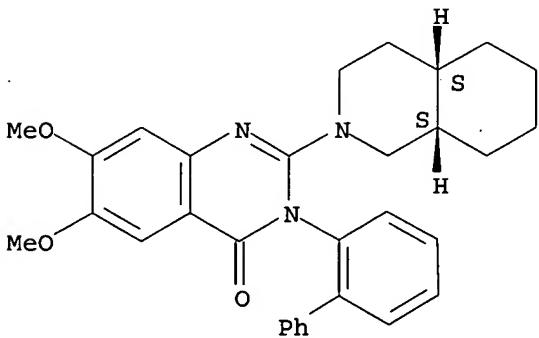
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L7 ANSWER 4 OF 5 CHEMCATS COPYRIGHT 2003 ACS  
Accession No. (AN): 2001:183634 CHEMCATS  
Catalog Name (CO): Chem.Folio  
Publication Date (PD): 15 May 2001 *Lat*  
Order Number (ON): TRG10400#06122-D  
Chemical Name (CN): 4 (3H)-Quinazolinone, 3-[1,1'-biphenyl]-2-yl-6,7-  
dimethoxy-2-[(4aR,8aR)-octahydro-2(1H)-isoquinolinyl]-  
, rel-  
CAS Registry No. (RN): 318957-11-8  
Supplementary Term (ST): CHEMICAL LIBRARY  
Structure :

Relative stereochemistry.



#### PRICES

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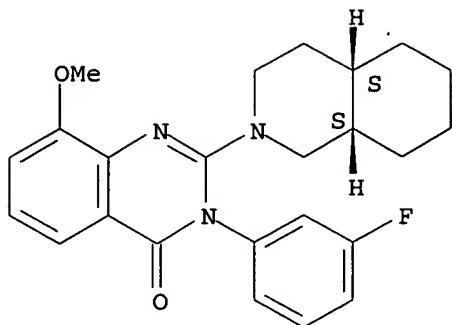
Phone: 858-410-6500  
Fax: 858-410-6501

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L7 ANSWER 5 OF 5 CHEMCATS COPYRIGHT 2003 ACS  
Accession No. (AN): 2001:183602 CHEMCATS  
Catalog Name (CO): Chem.Folio  
Publication Date (PD): 15 May 2001  
Order Number (ON): TRG10400#06032-D  
Chemical Name (CN): 4 (3H)-Quinazolinone, 3-(3-fluorophenyl)-8-methoxy-2-  
[(4aR,8aR)-octahydro-2(1H)-isoquinolinyl]-, rel-  
CAS Registry No. (RN): 318956-79-5  
Supplementary Term (ST): CHEMICAL LIBRARY  
Structure :

Relative stereochemistry.



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=> file caplus  
COST IN U.S. DOLLARS  
FULL ESTIMATED COST

SINCE FILE ENTRY	TOTAL SESSION
18.64	200.66

FILE 'CAPLUS' ENTERED AT 10:47:33 ON 31 MAR 2003  
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FILE COVERS 1907 - 31 Mar 2003 VOL 138 ISS 14  
FILE LAST UPDATED: 30 Mar 2003 (20030330/ED)

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=> d his

(FILE 'HOME' ENTERED AT 10:39:40 ON 31 MAR 2003)

FILE 'REGISTRY' ENTERED AT 10:39:58 ON 31 MAR 2003  
L1 STRUCTURE uploaded  
L2 0 S L1  
L3 9 S L1 FUL

FILE 'CAPLUS' ENTERED AT 10:40:38 ON 31 MAR 2003  
L4 0 S L3  
L5 3 S CAOLD

FILE 'CAOLD' ENTERED AT 10:41:37 ON 31 MAR 2003  
L6 0 S L3

FILE 'REGISTRY' ENTERED AT 10:42:11 ON 31 MAR 2003

FILE 'CHEMCATS' ENTERED AT 10:46:09 ON 31 MAR 2003  
L7 5 S L3

FILE 'CAPLUS' ENTERED AT 10:47:33 ON 31 MAR 2003

=> s 17  
L8 0 L3

=> file casreact  
COST IN U.S. DOLLARS  
FULL ESTIMATED COST

SINCE FILE ENTRY	TOTAL SESSION
0.83	201.49

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FILE CONTENT:1907 - 30 Mar 2003 VOL 138 ISS 13

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Crossover limits have been increased. See HELP RNCROSSOVER for details.

Structure search limits have been raised. See HELP SLIMIT for the new, higher limits.

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L9 0 L3

=> d his

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FILE 'REGISTRY' ENTERED AT 10:39:58 ON 31 MAR 2003  
L1 STRUCTURE uploaded  
L2 0 S L1  
L3 9 S L1 FUL

FILE 'CAPLUS' ENTERED AT 10:40:38 ON 31 MAR 2003  
L4 0 S L3  
L5 3 S CAOLD

FILE 'CAOLD' ENTERED AT 10:41:37 ON 31 MAR 2003  
L6 0 S L3

FILE 'REGISTRY' ENTERED AT 10:42:11 ON 31 MAR 2003

FILE 'CHEMCATS' ENTERED AT 10:46:09 ON 31 MAR 2003  
L7 5 S L3

FILE 'CAPLUS' ENTERED AT 10:47:33 ON 31 MAR 2003  
L8 0 S L7

FILE 'CASREACT' ENTERED AT 10:48:53 ON 31 MAR 2003  
L9 0 S L3

=> log y  
COST IN U.S. DOLLARS SINCE FILE TOTAL  
FULL ESTIMATED COST ENTRY SESSION  
25.80 227.29

STN INTERNATIONAL LOGOFF AT 10:49:53 ON 31 MAR 2003